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Guanidinium tin halide perovskites: structural, electronic, and thermodynamic properties by quantum chemical study

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Abstract

The orthorhombic phase of guanidinium tin halide perovskites $\text{C}(\text{NH}_2)_3\text{SnX}_3$, $\text{X} = \text{Cl}, \text{Br}, \text{I}$ has been studied by quantum chemical method. The lattice parameters are optimized to obtain the minimum energy using the density functional theory with the generalized gradient approximation, GGA-PBE. The Kohn–Sham electronic band structures have been computed; the materials have direct bandgaps of 3.00, 2.47, and 1.78 eV for the $\text{C}(\text{NH}_2)_3\text{SnCl}_3$, $\text{C}(\text{NH}_2)_3\text{SnBr}_3$, and $\text{C}(\text{NH}_2)_3\text{SnI}_3$, respectively, situated at the gamma symmetry points. The projected densities of states are analyzed and the contribution of the p- and s-states of the tin and halogen atoms evaluated. For the GUASnX_3 compounds, thermodynamic stability to different decomposition routes has been assessed and standard enthalpies of formation obtained.

Keywords

Guanidinium; Lead-free; Enthalpy of formation; The density of states; Orthorhombic; Bandgap